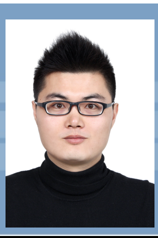
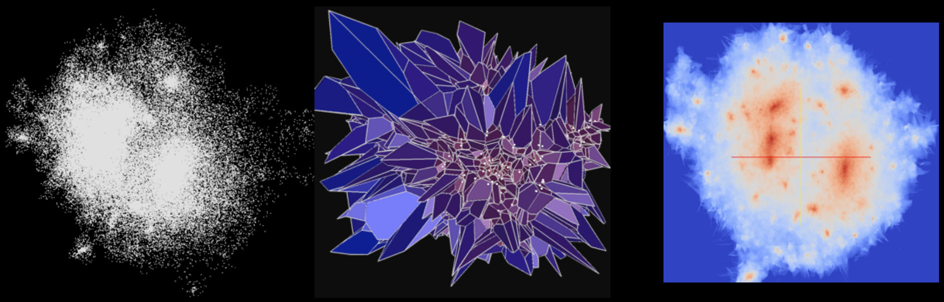
  

Adaptive Density Estimation of Particle Data

Tom Peterka[1], Steve Rangel[2], Nan Li[3],
Salman Habib[1], Katrin Heitmann[1]

[1]Argonne National Laboratory
[2]Northwestern University
[3]University of Chicago

Halo particles, Voronoi tessellation, and 2D density estimation



Tom Peterka
tpeterka@mcs.anl.gov
Mathematics and Computer Science Division

CoDA Invited Talk
3/5/14

Executive Summary

We describe work in progress for sampling a regular density field from a distribution of particle positions using a Voronoi tessellation as an intermediate data model.

Key Ideas

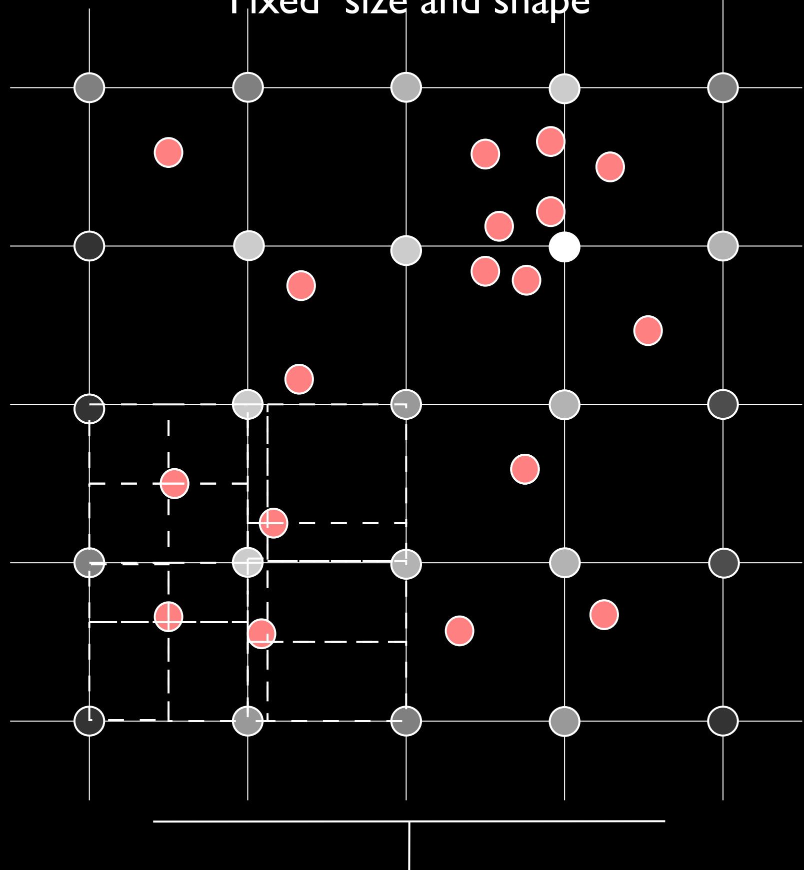
- Convert discrete particle data into continuous function that can be interpolated, differentiated, interpolated, represented as a regular grid (field)
- Automatically adaptive window size and shape
- Comparison with CIC and SPH using synthetic and actual data
- Voronoi tessellation and density estimation computed in parallel on distributed-memory HPC machines
- Application to gravitational lensing

Preliminaries

Estimation Kernels

CIC

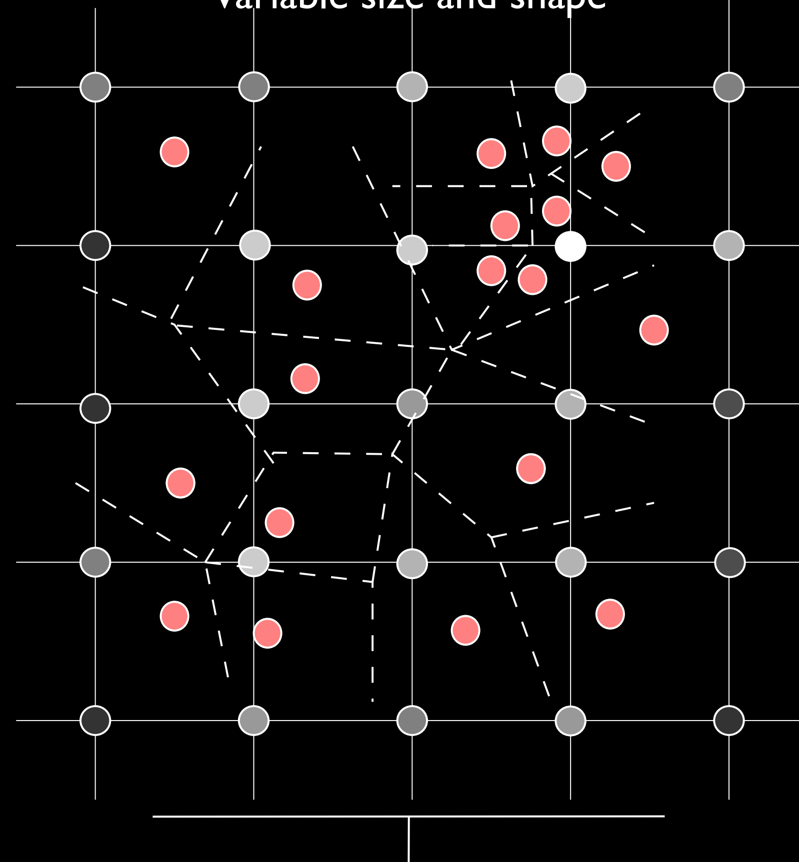
Fixed size and shape



In cloud-in-cell (CIC) methods, particles are distributed to a fixed number of grid points.

TESS

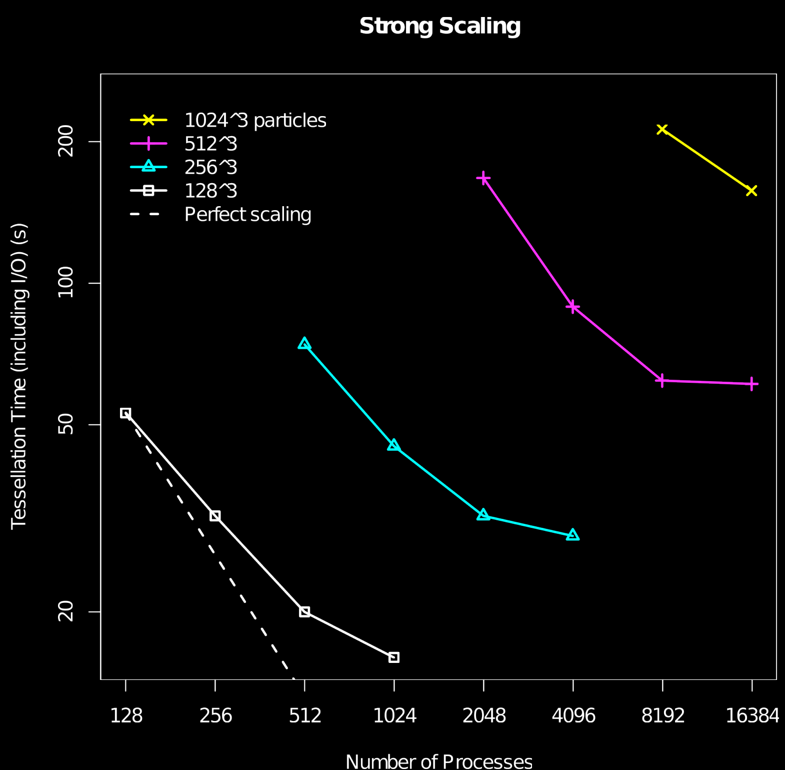
Variable size and shape



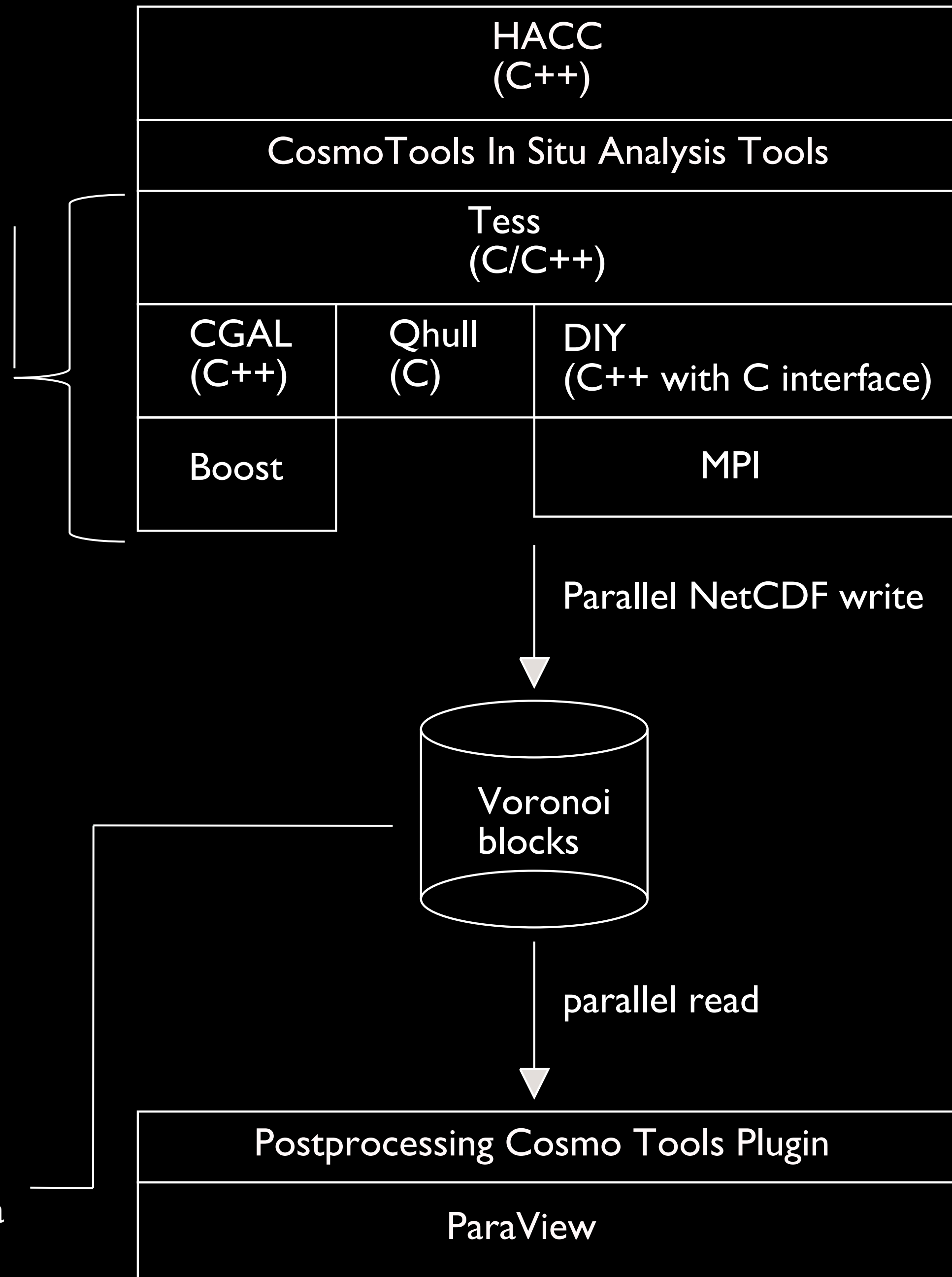
In tessellation (TESS) methods, particles are distributed to a variable number of grid points according to the Voronoi or Delaunay tessellation that has variable size and shape cells.

Tess Library

Tess is our parallel library for large-scale distributed-memory Voronoi and Delaunay tessellation.



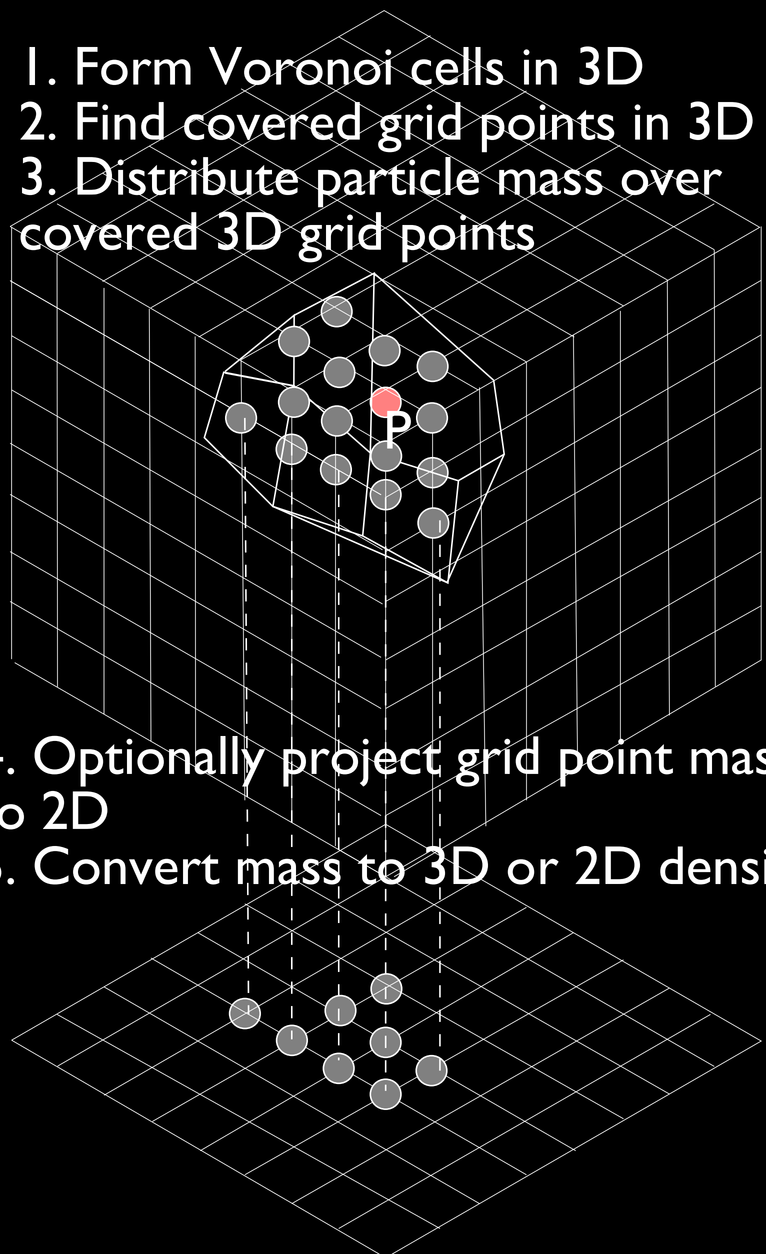
Dense, our density estimator, currently reads the tessellation from disk and estimates density onto a regular grid. Eventually dense will be converted to a library that can be coupled in memory to tess output, saving the tessellation storage.



Method

Overall Algorithm

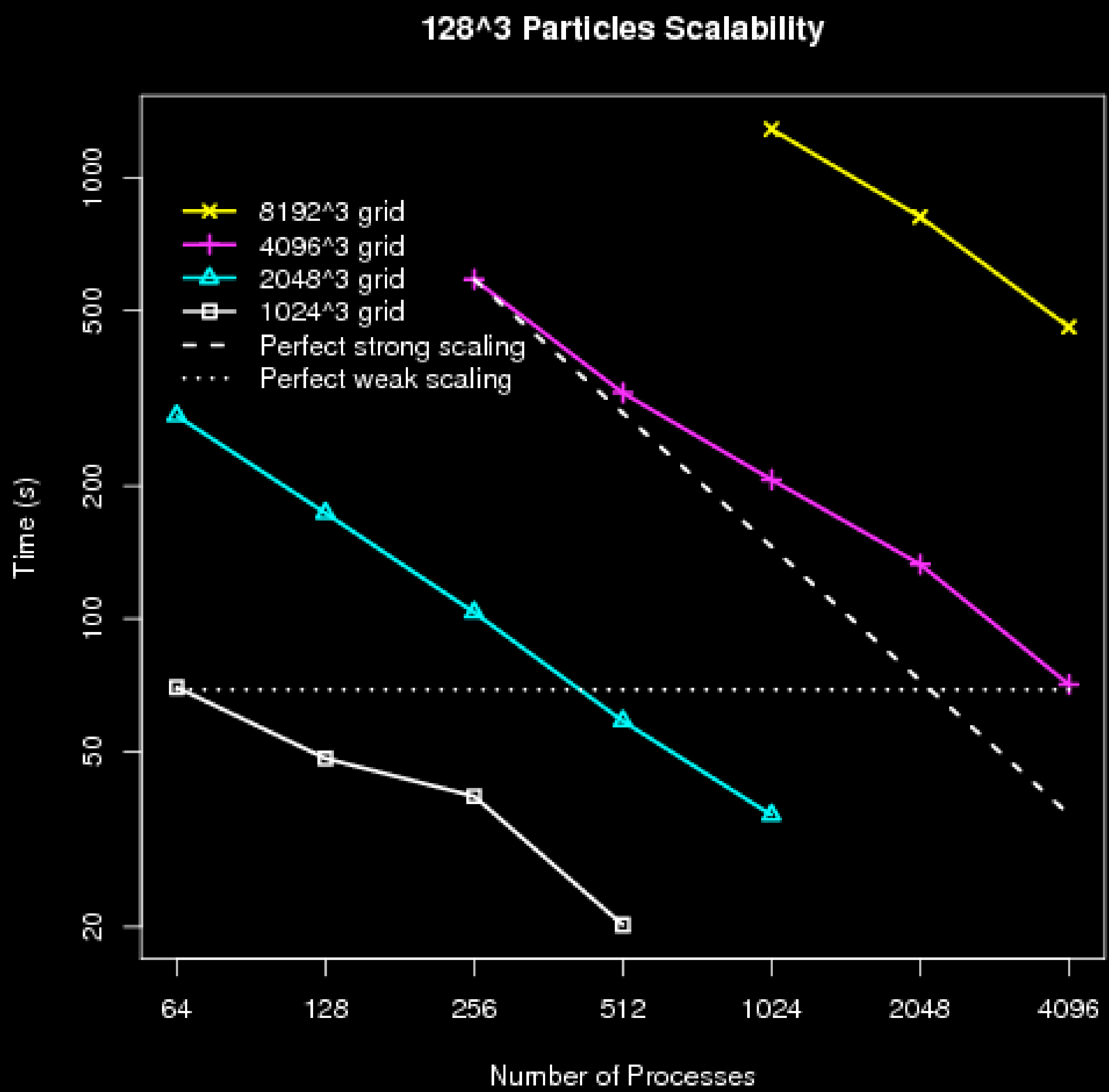
1. Form Voronoi cells in 3D
2. Find covered grid points in 3D
3. Distribute particle mass over covered 3D grid points
4. Optionally project grid point mass to 2D
5. Convert mass to 3D or 2D density




```
for (all Voronoi cells) {

  compute grid points in cell bounding box

  compute Voronoi cell interior grid points from
     grid points in cell bounding box

  for (all interior grid points) {

    if (grid point is in bounds of local block)
      add mass contribution to grid point

    else
      send mass contribution to neighboring block
         containing grid point and add it there

    if (no grid points in interior of Voronoi cell)
      add mass contribution to single nearest
         grid point

    if (2D projection) {
      accumulate mass at 2D pixel
      divide by pixel area for 2D density
    }

    else
        divide by voxel volume for 3D density

  } // interior grid points

} // Voronoi cells
```

Dense Strong and Weak Scaling

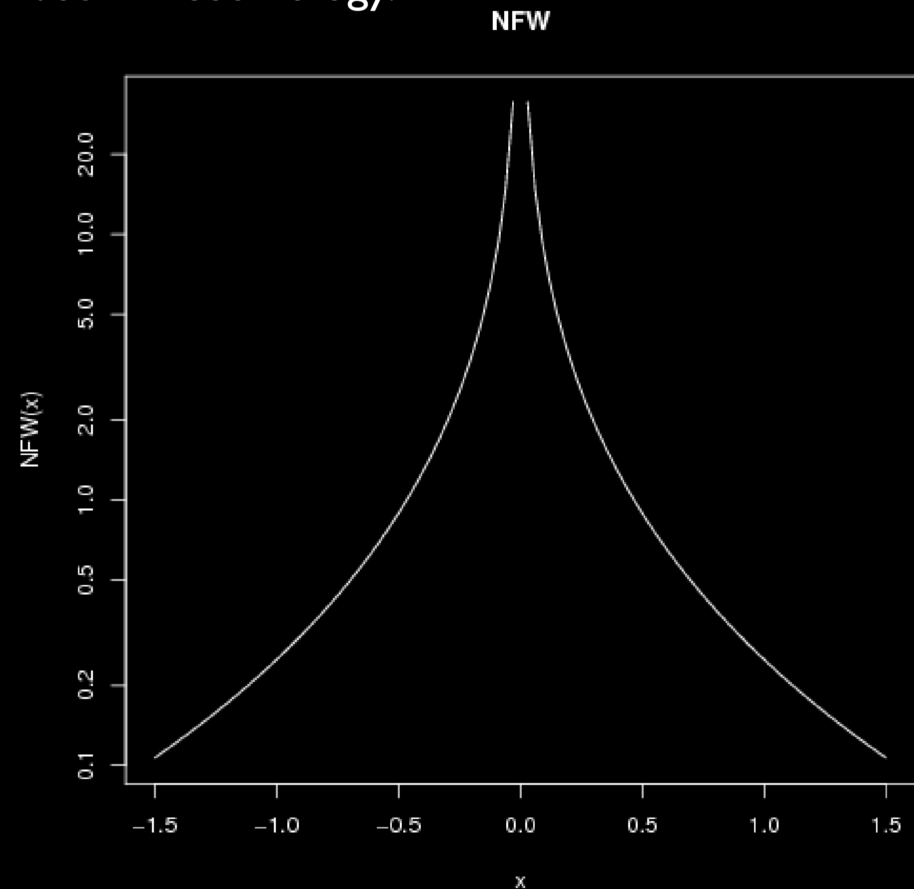
- 128^3 synthetic particles
- End-to-end time (including reading tessellation and writing image)
- 3D->2D projection
- 51% strong scaling (End-to-end) for 4096^3 grid



Accuracy

Navarro-Frenk-White (NFW)

Our first synthetic dataset is derived from an analytical density function commonly used in cosmology.



k is a constant, 1 for us

$\rho\,(r)$ is Monte Carlo sampled to get test set of particles

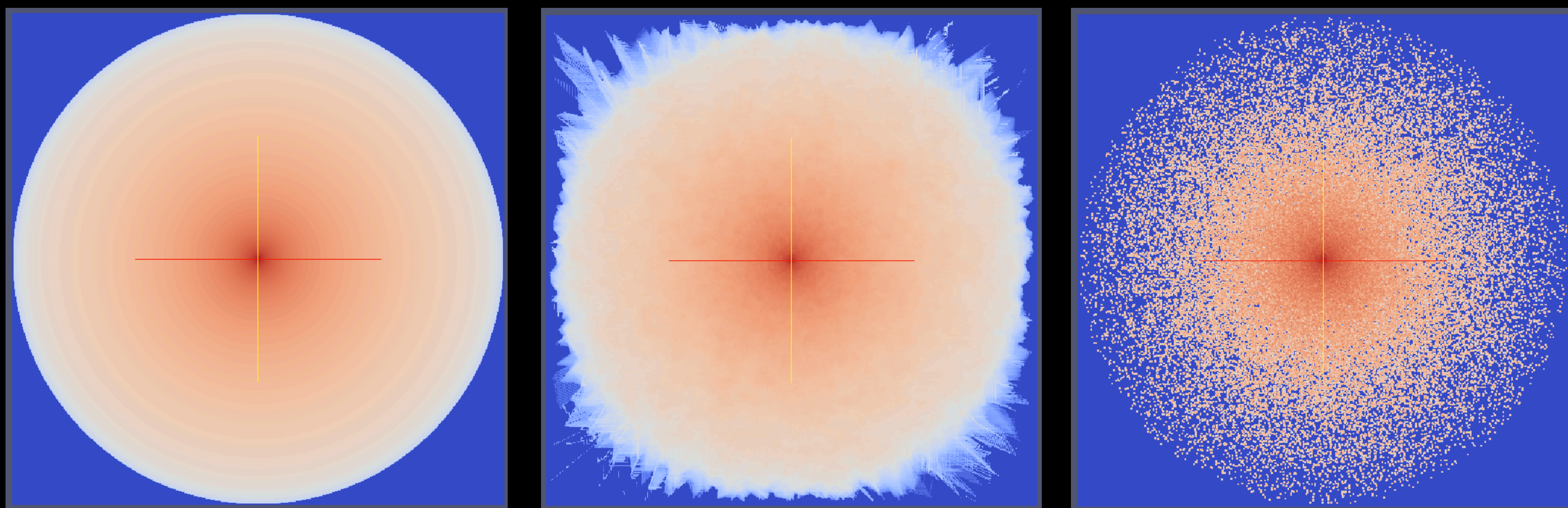
Ground truth is 2D plot of $\rho\,(r)$

We limit r to [-1.5, 1.5] and NFW(r) to 10^6

$$\rho(r) = \frac{k}{(r(r+1)^2)}$$

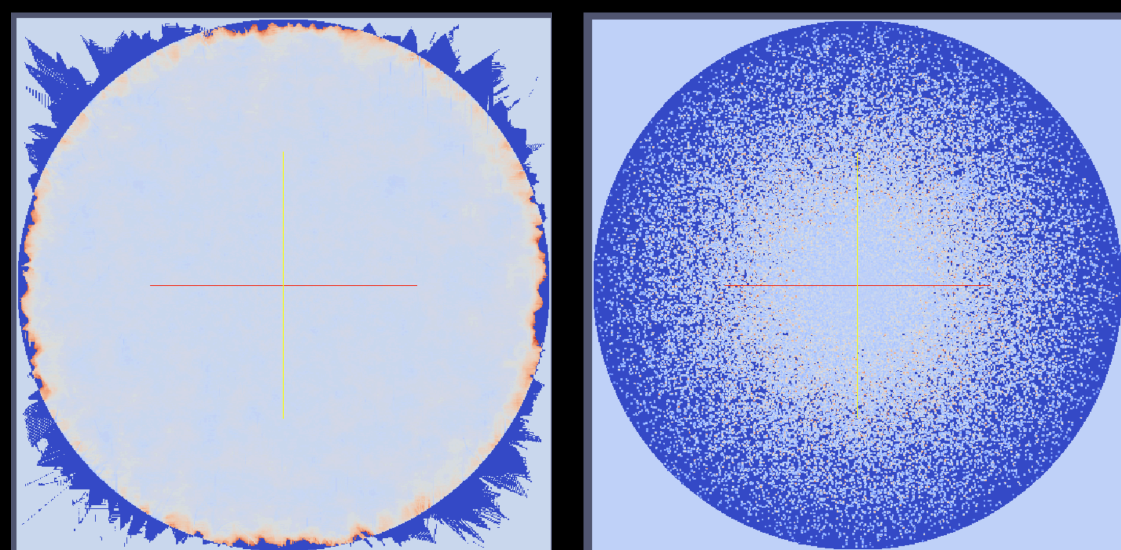
NFW 2D Density Fields

Analytical TESS CIC



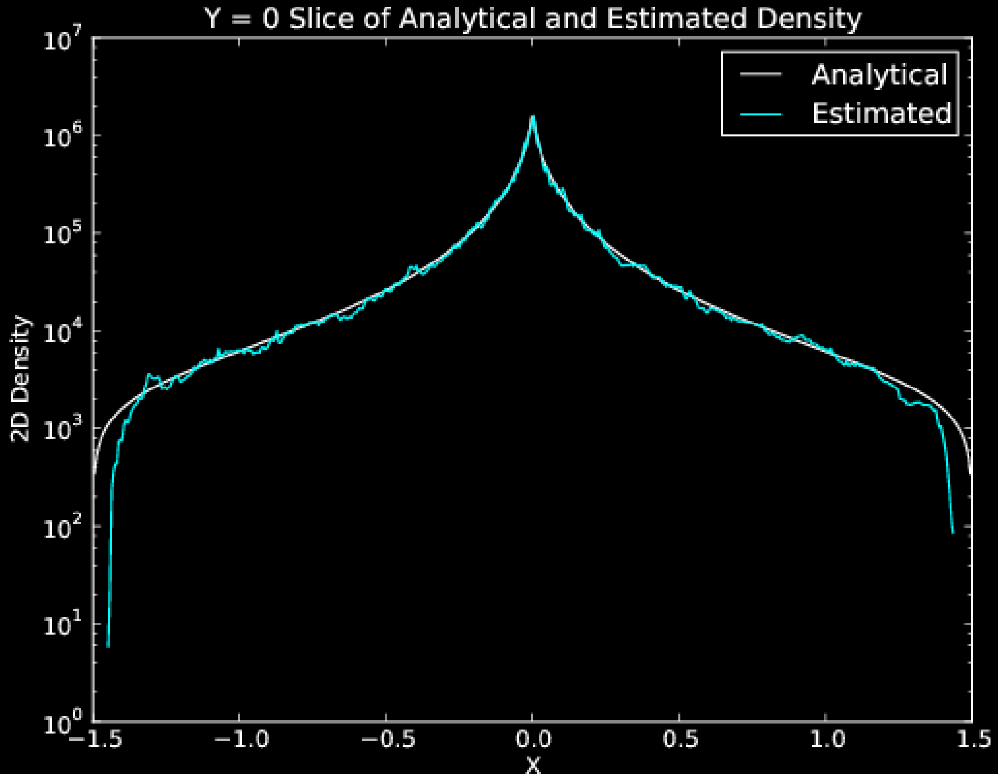
Top row:
1024^3 3D density projected to 1024^2 2D density field and rendered in ParaView

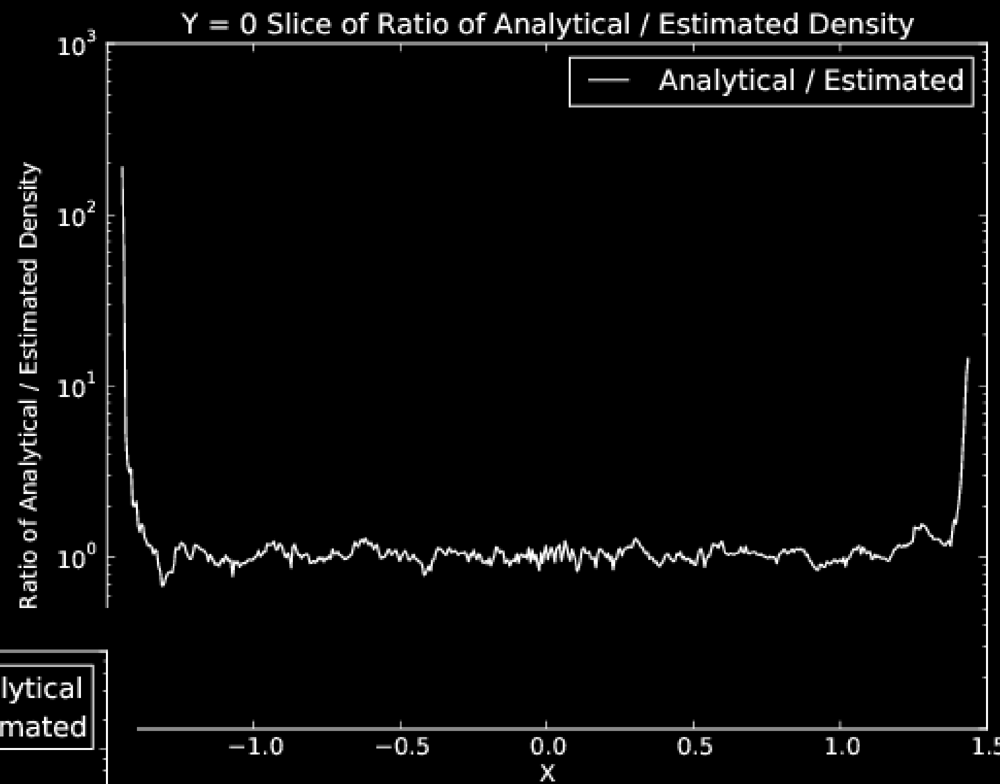
Bottom row:
Ratio of analytical divided by estimated density



TESS

Comparison between analytical 2D density and estimated density at $y = 0$ cross section

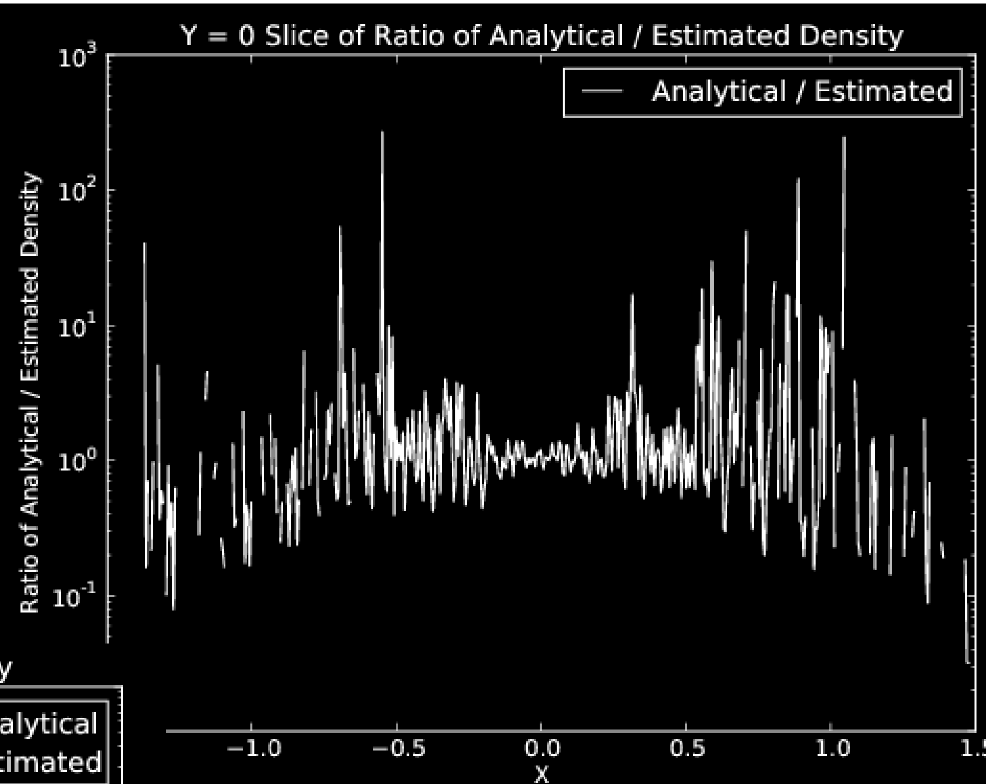


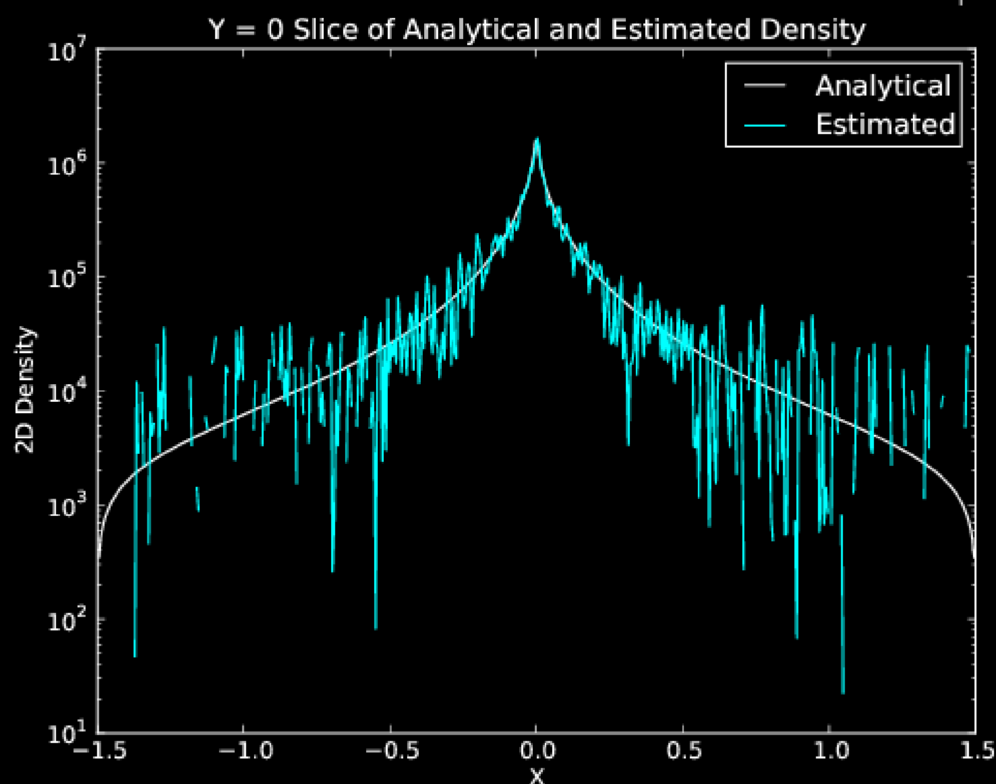


Ratio between analytical 2D density divided by estimated density at $y = 0$ cross section

CIC

Comparison between analytical 2D density and estimated density at $y = 0$ cross section

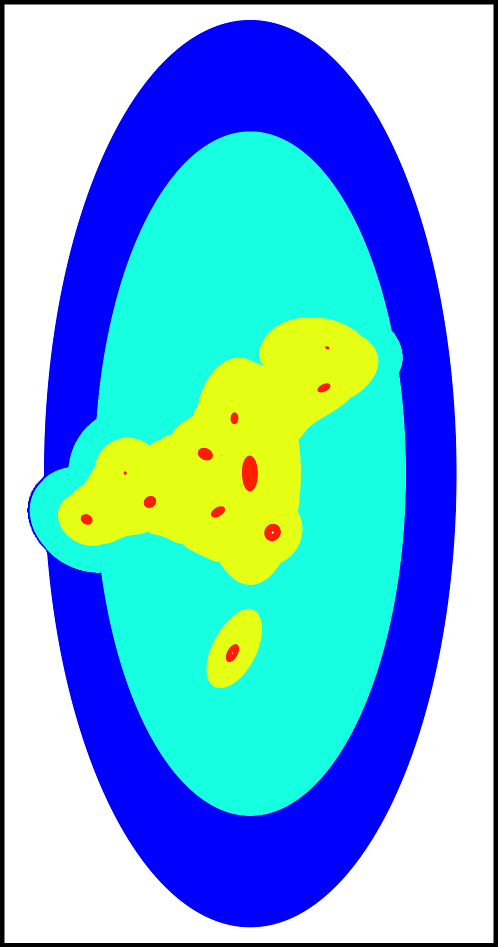




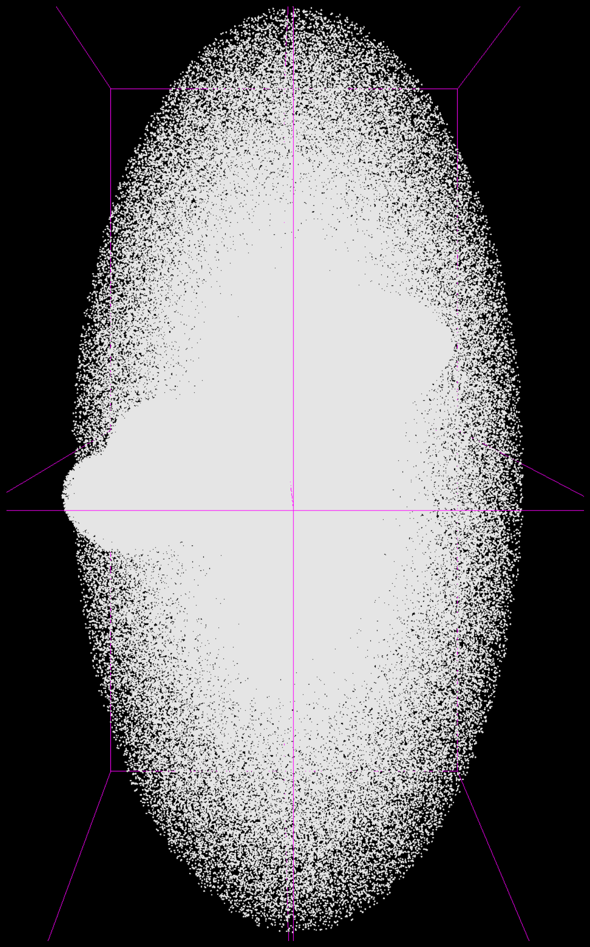
Ratio between analytical 2D density divided by estimated density at $y = 0$ cross section

Complex NFW (CNFW)

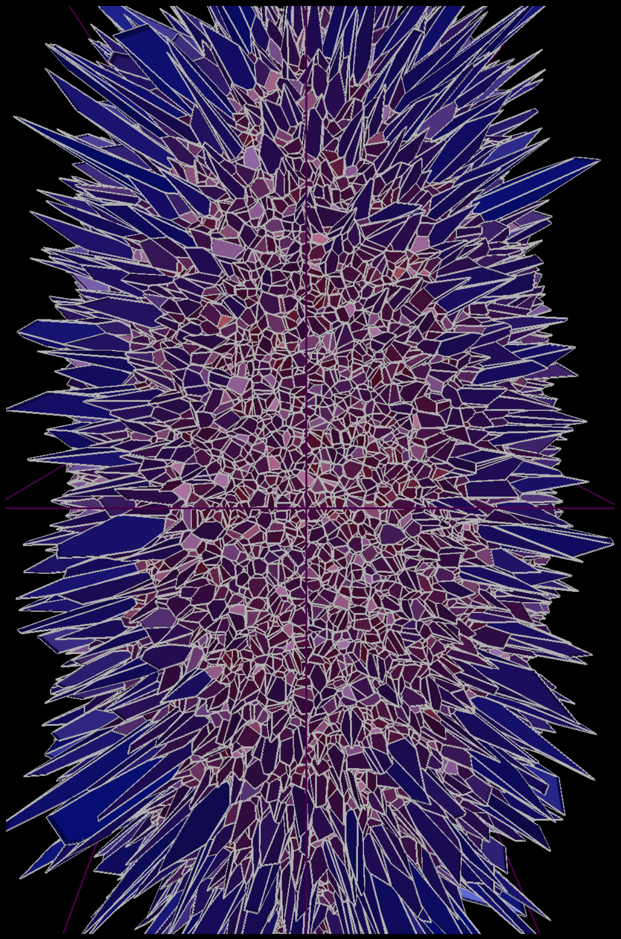
Our second synthetic dataset is a combination of several NFWs of varying cutoff densities and asymmetric scaling factors.



Analytical cutoff density contours

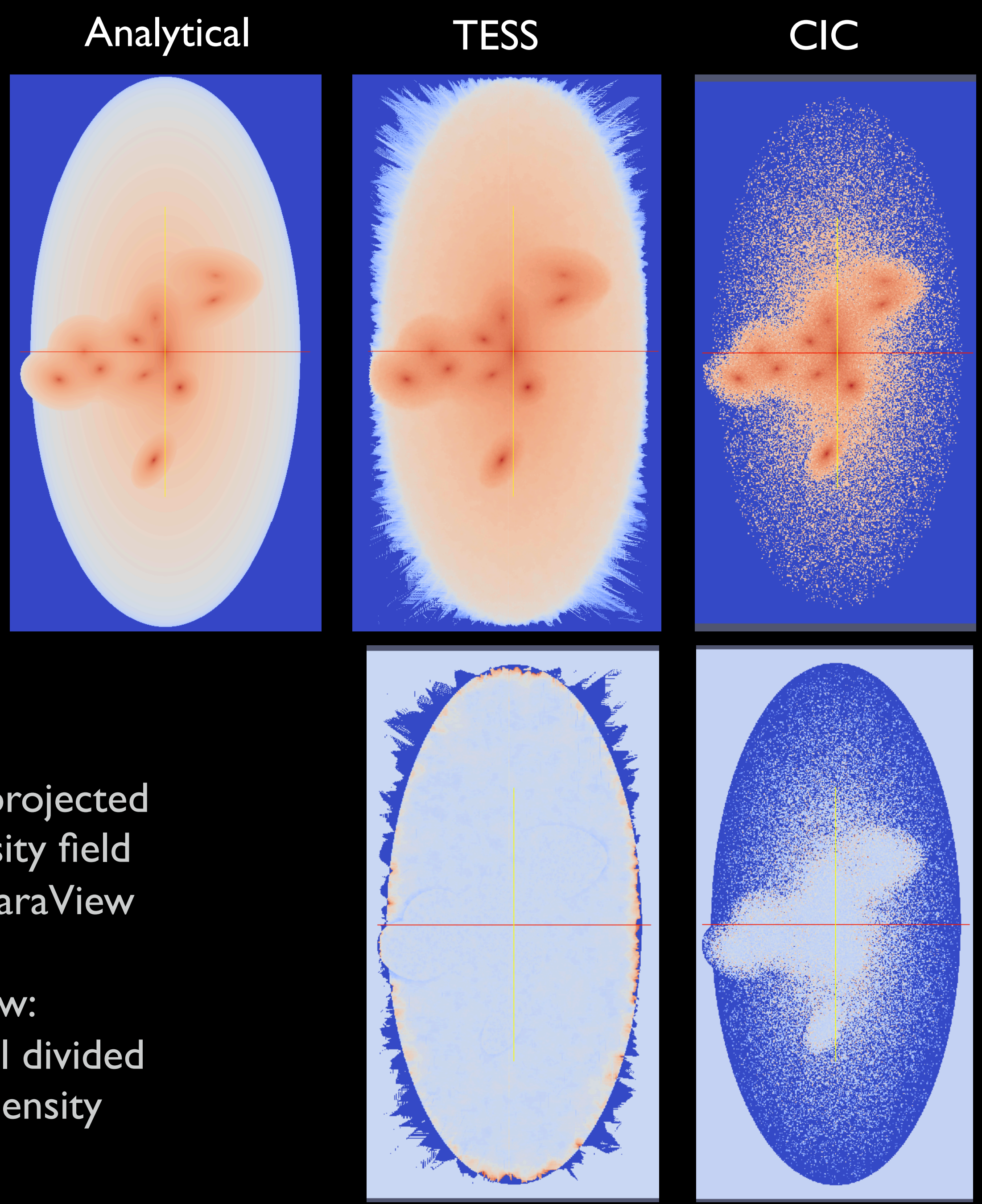


2e5 sampled particles



Voronoi tessellation

CNFW 2D Density Fields

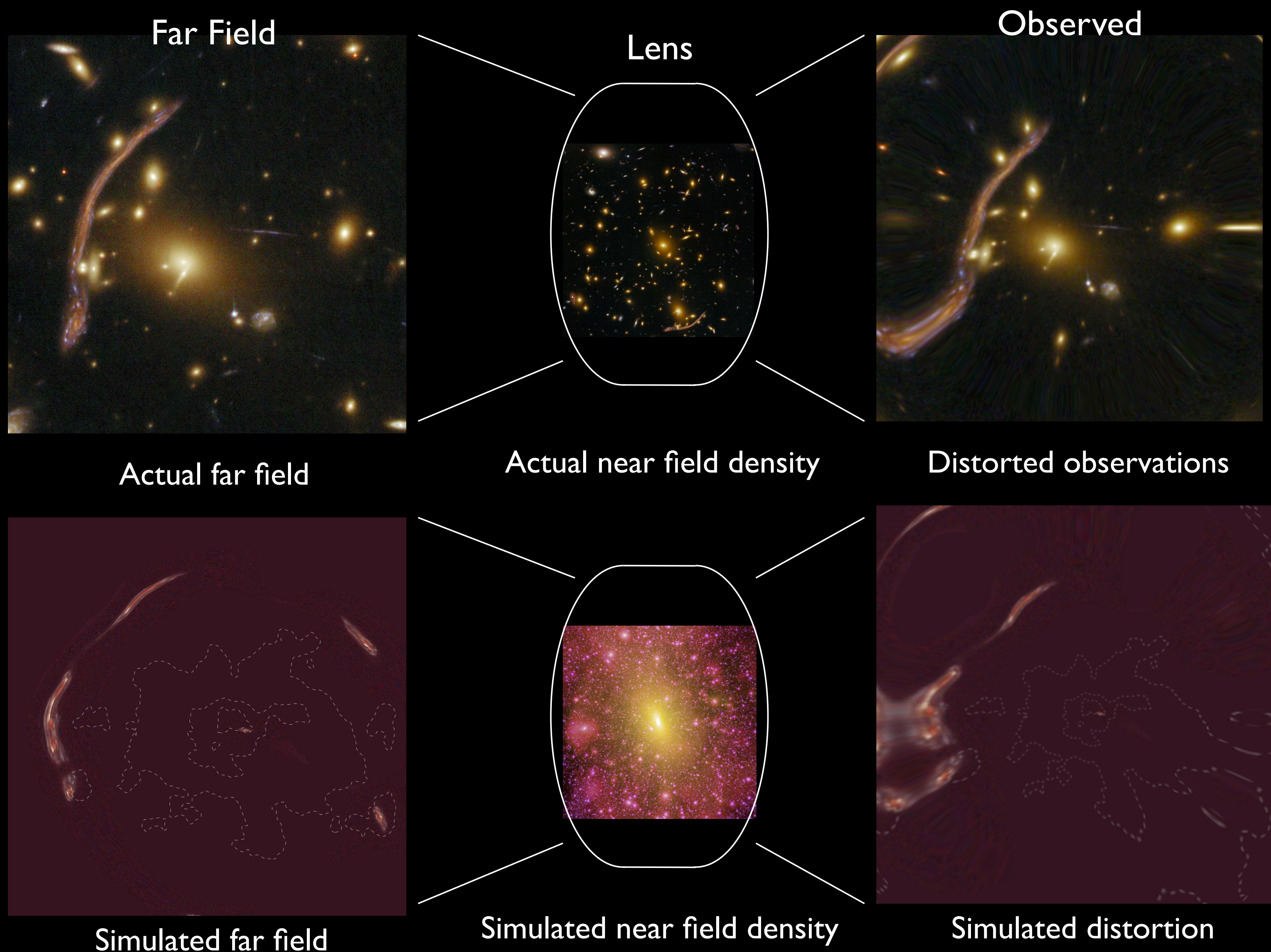


Top row:
1024^3 3D density projected to 1024^2 2D density field and rendered in ParaView

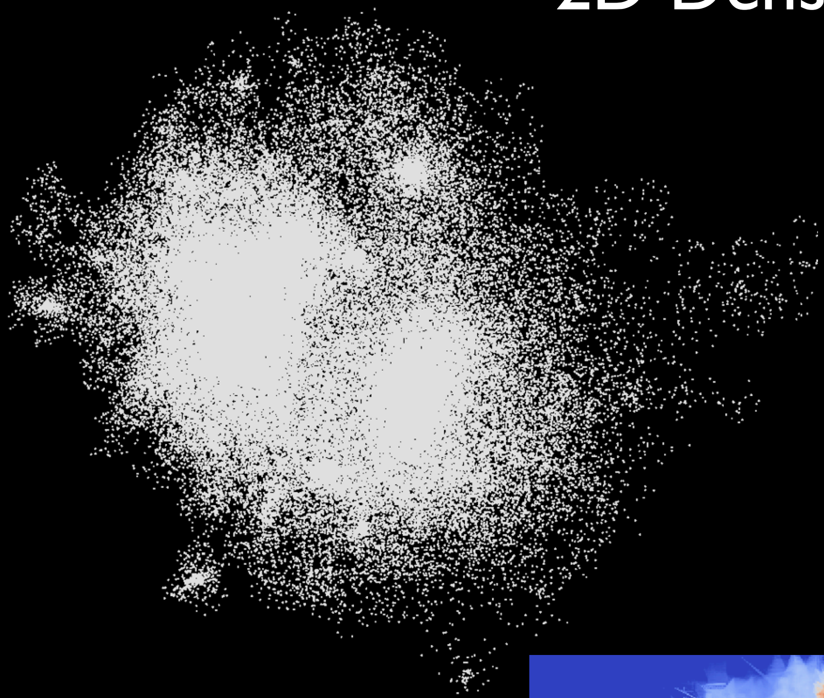
Bottom row:
Ratio of analytical divided by estimated density

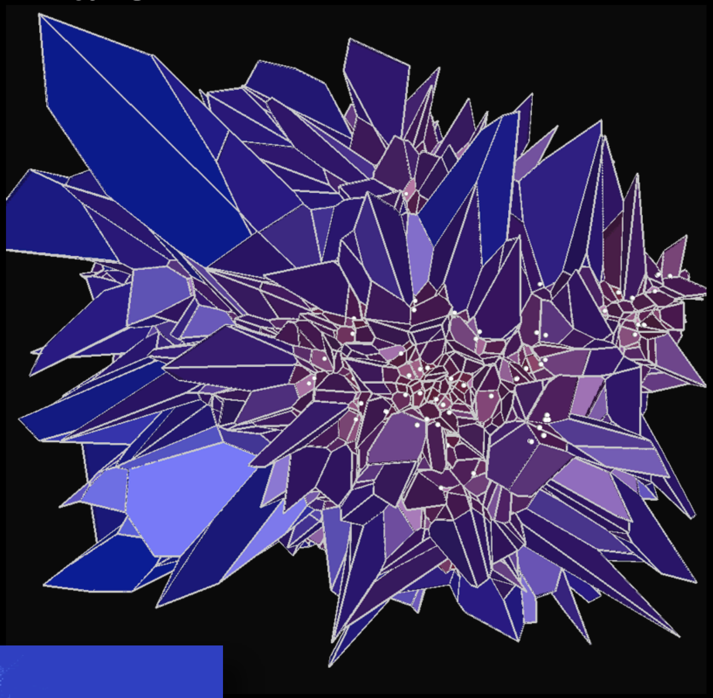
Application: Gravitational Lensing

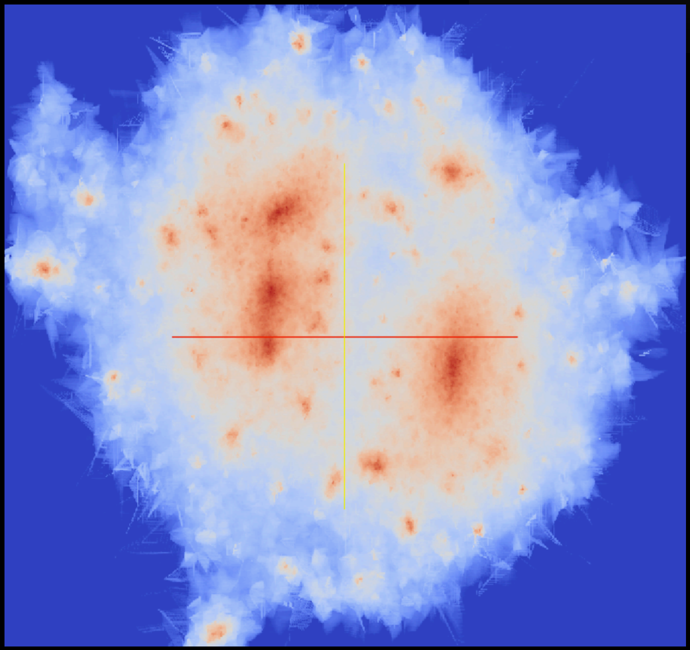
Lensing for Validating Simulations with Sky Surveys



2D Density of Halo







Particle data from HACC N-body cosmology code from halo ID 7445077095

Voronoi tesellation of halo particles colored by cell volume

Final output 2D density field for lensing

Summary

I described sampling a regular density field from a distribution of particle positions using a Voronoi tessellation as an intermediate data model.

Key Ideas

- Automatically adaptive window size and shape
- Comparison with CIC and SPH using synthetic and actual data
- Voronoi tessellation and density estimation computed in parallel on distributed-memory HPC machines
- Application to gravitational lensing

Ongoing and Future Work

- Linear Barycentric interpolation inside Voronoi cells through Delaunay tessellation
- Shared memory threading inside MPI tasks
- Other applications such as 3D volume rendering

“The purpose of computing is insight, not numbers.”

–Richard Hamming, 1962

Acknowledgments:

Facilities

Argonne Leadership Computing Facility (ALCF)

Funding

US DOE SciDAC SDAV Institute

People

Juliana Kwan, Hal Finkel, Adrian Pope, Nick Frontiere, George Zagaris

Software

https://repo.anl-external.org/repos/tess/trunk

CoDA Invited Talk
3/5/14

Tom Peterka

tpeterka@mcs.anl.gov

Mathematics and Computer Science Division